SOS 10
Capability Machines Panel

Al Geist
Oak Ridge National Laboratory
Oak Ridge, TN U.S.A

SOS 10 Conference
Maui, Hawaii
March 7, 2006

Research sponsored by U.S. Department of Energy

1. Describe the Capability Resources at your site (ORNL)

ornl

25.1 TF Cray XT3 (scalar)

- 2 GB memory per processor
- 11 TB aggregate memory
- 120 TB disk space
- 5,294 processors
- 56 cabinets

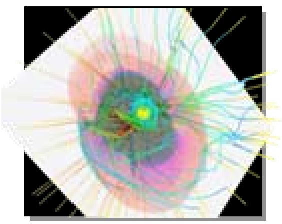
18.5 TF Cray X1E (vector)

- Most powerful X1E in world
- 2 TB globally shared memory
- 32 TB disk space
- 1,024 processors
- 12.8 GF per CPU
- 34.1 GB/s main memory BW

5 PB HPSS storage system

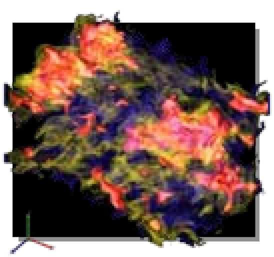
2. Describe applications where your unique capability platform was critical to solution

Examples that used Cray X1E:



3D Studies of Stationary Accretion Shock Instabilities in Core Collapse Supernovae

Simulations have uncovered a new instability of the shock wave and a resultant spin-up of the stellar core beneath it, which may be integral to reenergizing the shock and explain key observables such as neutron star "kicks" and the spin of newly-born pulsars.



Turbulent Premix Combustion In Thin Reaction Zones

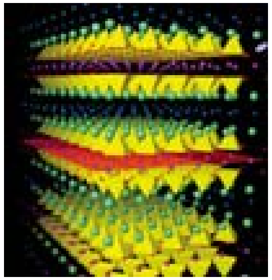
Calculations show the importance of considering the interplay of diffusion and reaction, particularly where strong finite-rate chemistry effects are involved.

Full Configuration Interaction Benchmarks for Open Shell Systems

Large, fast computational power enable advancement from approximate to exact models of molecules, especially for complex open-shell systems and excited states.

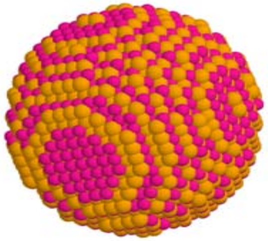
2. Describe applications where your unique capability platform was critical to solution

Examples that used Cray XT3:



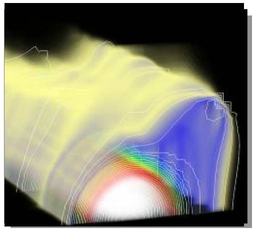
Resolving Material Disputes

A recent *Nature Materials* article used the results from simulations on Jaguar to resolve long-standing discrepancies between phenomenological models, widely used to describe properties of new semiconductor materials, and first-principles electronic structure descriptions of magnetic semiconductors.



Smaller is Better

By engineering nanoparticles' size, shape and surface chemistry, the capacity for information storage can be increased dramatically in comparison to bulk materials. Over 81% of theoretical peak performance was achieved for the non-collinear magnetic structure calculation of FePt particles containing up to 2662 atoms.

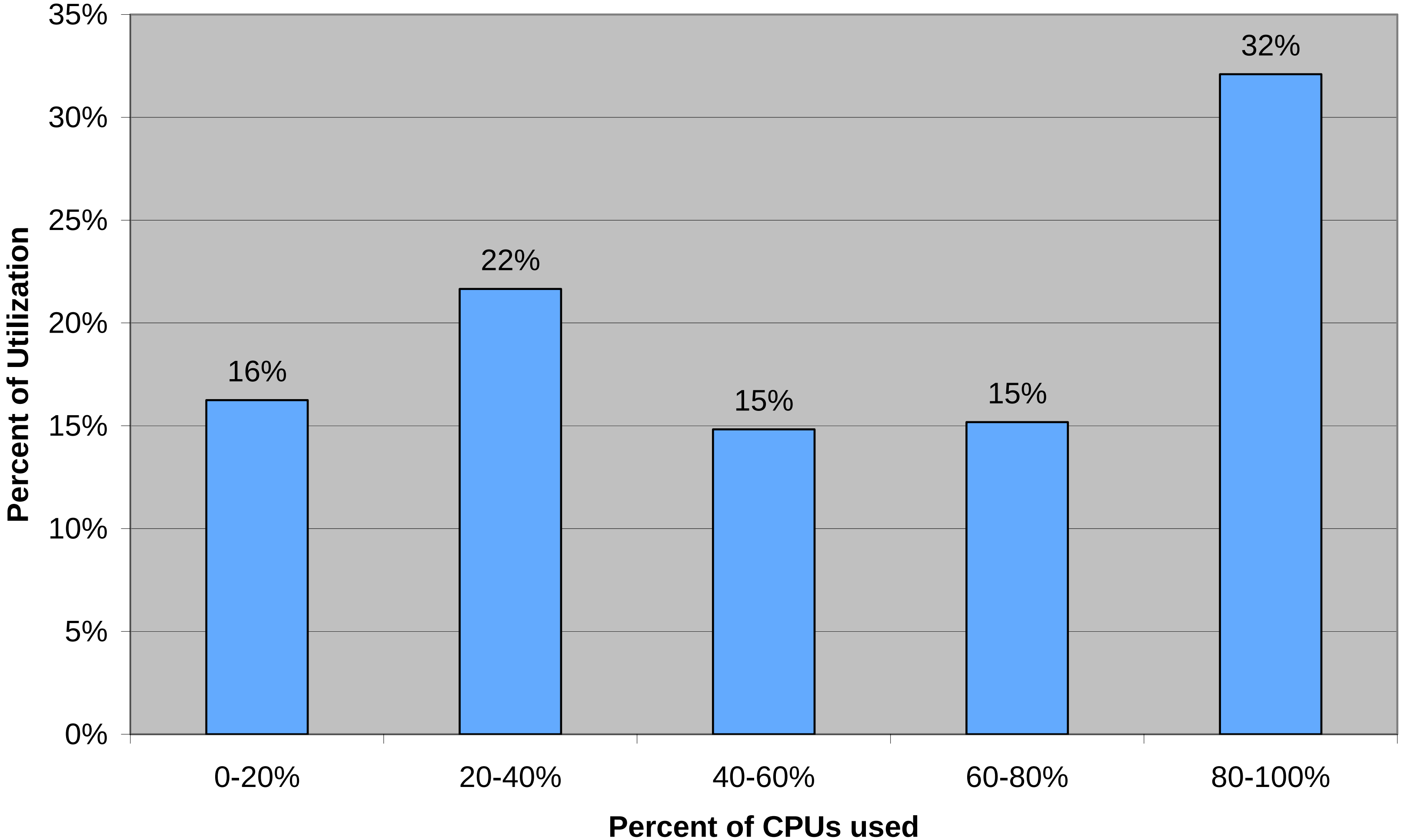


Plasma Turbulence

Simulations of the turbulence and flow of plasma is critical for developing tools to harness and use the power from fusion reactions and to address astrophysical challenges such as solar-coronal mass ejections.

- **Calculations carried out weeks after delivery of Jaguar**
- **Largest-ever simulation of plasma behavior in a tokamak**
- **Simulation used 3072 processors (roughly 60% of the entire system)**

Over 30% of jobs use more than 80% of 5,200 proc on XT3



Scientist will take advantage of large system if available and make new discoveries.

3. What is the Distinction between Capability and Capacity

Don’t agree with metrics defined in the abstract i.e.

Capability metric – time to solution

Capacity metric – sustained performance per unit cost

Capability computing is a valuable, scarce resource typically used by a “small” number of people per year

Capability

Hubble $1.5B

Capacity

5 million Binoculars $1.5 B

Focused on calculations or simulations of high scientific impact not possible to do otherwise

4. Is the Distinction Useful?

Yes, if we get the definition right.

It helps define a use model

And by analogy to other scientific instruments it helps define a review process of determining which science proposals will get access to the scarce resource(s)

No one architecture is ideal for all science applications.

Ideally the results (data) would be publicly available to the entire scientific community

5. What metrics do you use to measure capability?

ornl

A capability scientific instrument is a valuable, scarce resource only able to be used by a “small” number of people per year, eg. accelerator, telescope, mars rover…

To maximize scientific impact we are trying to set up a computation resource or set of resources at a limited number of sites as capability scientific instruments focused on calculations or simulations of high scientific impact not possible to do otherwise

The metrics for scientific instruments is the high quality science that they enable often measured by the community’s perception of impact and/or prestige of papers produced.

Questions?

Backup Slides

NCCS Resources

September 2005 Summary

Network Routers

Control Network
1 GigE
10 GigE
UltraScience

Cray XT3 Jaguar	Cray X1E Phoenix	SGI Altix Ram	IBM SP4 Cheetah	IBM Linux NSTG	Visualization Cluster	IBM HPSS
						
(5,294) 2.4GHz 11TB Memory	(1,024) 0.5GHz 2 TB Memory	(256) 1.5GHz 2TB Memory	(864) 1.3GHz 1.1TB Memory	(56) 3GHz 76GB Memory	(128) 2.2GHz 128GB Memory	Many Storage Devices Supported
120TB	32TB	36TB	32TB	4.5TB	9TB	5TB

Shared Disk: 120TB, 32TB, 36TB, 32TB, 4.5TB, 9TB, 5TB

Backup Storage: 5PB

Summary

- 7 Systems
- Supercomputers: 7,622 CPUs, 16TB Memory, 45 TFlops
- 238.5 TB
- 5 PB

Scientific Visualization Lab
- •27 projector Power Wall

Test Systems
- •96 processor Cray XT3
- •32 processor Cray X1E*
- •16 Processor SGI Altix

Evaluation Platforms
- •144 processor Cray XD1 with FPGAs
- •SRC Mapstation
- •Clearspeed
- •BlueGene (at ANL)